Internship & PhD proposal: Uncertainty quantification for the closure modeling of the turbulent Reynolds stress tensor

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Scientific context

This position is a part of the ANR project Exa-MA (Methods and Algorithms for Exascale) dealing with high-performance computing methods and its adaptation to the forthcoming so-called exascale hardware. This combined internship and PhD proposal concerns UQ (Uncertainty Quantification) developments on turbulence closure modeling for CFD (Computational Fluid Dynamics). The *Commissariat à l'énergie atomique* (CEA) will bring expertise on applied statistics and turbulence closure modeling whereas *l'École Nationale de la Statistique et de l'Analyse de l'Information* (ENSAI) will bring sound mathematical tools for uncertainty quantification.

The intern-then-PhD student will be mainly based in CEA Saclay research center, in the outskirts of Paris, with several meetings in the ENSAI Campus near Rennes. It will be supervised by Clément Gauchy and Pierre-Emmanuel Angeli in CEA, and Sébastien Da Veiga in ENSAI who will be the PhD director.

Description and objectives

Turbulence closure modeling and the peculiar role of the Reynolds stress tensor

Turbulence effects arise in many engineering applications with high level of performance and safety standards. Accurate predictions of turbulent flows are of vital importance especially for the nuclear industry. The dynamic of fluid flows is governed by the famous Navier-Stokes (NS) equations. In the context of incompressible incompressible Newtonian flows of constant property, the NS equations writes:

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{\mathrm{Re}}\frac{\partial^2 u_i}{\partial x_j^2} \quad (2)$$

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where $u_i,\ p,\ x_i,\ t$ are respectively the flow velocity, the pressure field, the spatial coordinate and the time. The Reynolds number Re measures the relative importance of inertia to viscous forces. The higher the Reynolds number, the more chaotic are the solutions of the NS equations. The flow velocity field then exhibits strong fluctuations that are characteristic of the turbulent regime and drived by the nonlinear convection terms $\partial u_i u_j / \partial x_j$.

Direct Numerical Simulations (DNS) requires a very fine meshing to provide an admissible numerical of the solution of the NS equations, implying a intractable computational time with respect to industrial constraints. The Reynolds-Averaged Navier-Stokes (RANS) equations provides faster numerical computations while conserving a good representation of the turbulent flows. It is based on the decomposition of the flow velocity field as by a mean component and a fluctuating component:

$$u_i = \langle u_i \rangle + u_i'$$

with the following assumption that $\partial \langle u_i \rangle / \partial t = 0$. Applying the mean operator and by incorporating this decomposition into the NS equations allows us to write the following equations:

$$\frac{\partial \langle u_i \rangle}{\partial x_i} = 0 \tag{3}$$

$$\langle u_i \rangle \frac{\partial \langle u_j \rangle}{\partial x_j} = -\frac{\partial \langle p \rangle}{\partial x_i} + \frac{1}{\mathrm{Re}} \frac{\partial^2 \langle u_i \rangle}{\partial x_j^2} - \frac{\partial \langle u_i' u_j' \rangle}{\partial x_j} \tag{4}$$

This formulation is called the RANS formulation of the NS equations. The equations become stationary but with a new source term, the **Reynolds stress tensor** (RST) $\tau_{ij} = -\langle u_i' u_j' \rangle$. Turbulence closure modeling is dedicated to finding a model for the RST that can be based on both physical arguments and experimental measurements. The determination of the RST *via* turbulence closure modeling is critical for solving the RANS equations. Moreover, due to the importance of the simulation of turbulence effects for industrial applications, research on uncertainty quantification methodologies on the RST have been heavily developed in the recent years [8, 7].

Objectives

The main objective of the PhD is to develop an uncertainty quantification framework for the RST modeling. Here are some potential and non-exhaustive research axes:

- Gaussian process regression is oftenly used in uncertainty quantification due to its ability to provide both a prediction and an uncertainty on its prediction. Also known as kriging, it is also used in spatial stastistics. Gaussian process regression extensions for tensor prediction has already been studied for the determination of stress tensors of hyperelastic materials [1, 4]. However, Reynold stress tensors form a spatial tensor field and the spatial correlation has to be taken into account while being computationally tractable. Specific algorithms for training and sampling the Gaussian process posterior distribution will be derived using advanced tools coming from the spatial statistics literature (e.g. Vecchia approximation [6], Fast Fourier transform,...).

- Uncertainty quantification will be performed on the Reynold stress tensor spatial field. The main challenge will consists in developing a sound mathematical framework to statistically describe the RST field. While central and dispersion statistics such as mean and variance are straightforward for a tensor spatial field, risk statistics such as quantile or superquantile are not easily defined for random variable of dimension more than one. A new notion of multivariate quantile based on Optimal Transport (OT) has been recently introduced [5] along with recent developments of efficient estimation algorithms [3, 2].

Wished profile, salary, duration

The ideal candidate should have confirmed skills in probability theory and statistics, as well as some background knowledge in fluid dynamics and/or applied physics.

The internship before the start of PhD will be about **6 months duration**, starting any time after **March 2024**, with **a monthly salary between 700€ and 1300€ depending on the candidate's profile, as well as an housing assistance of about 200€**.

The PhD will start by any time between **September and December 2024**. It is a **three years contract with a gross annual salary around 28.5k€ (independent of the candidate's profile).**

For both the internship and the PhD, **there is an financial assistance of 75% of the public transport subscription fees**.

CEA offers to their employees a free bus shuttle service from a variety of places in Île-de-France region to reach the CEA Saclay research center more easily. Ask us to have more details on the different shuttle lines and timeschedules!

If you feel interested by the proposal, please get in touch by e-mail with C. Gauchy, P-E. Angeli and S. Da Veiga.

References

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